

Quantum response of finite Fermi systems and the relation of Lyapunov exponent to transport coefficients

Klaus Morawetz

Fachbereich Physik, University Rostock, D-18055 Rostock, Germany

Within the frame of kinetic theory a response function is derived for finite Fermi systems which includes dissipation in relaxation time approximation and a contribution from additional chaotic processes characterized by the largest Lyapunov exponent. A generalized local density approximation is presented including the effect of many particle relaxation and the additional chaotic scattering. For small Lyapunov exponents relative to the product of wave vector and Fermi velocity in the system, the largest Lyapunov exponent modifies the response in the same way as the relaxation time. Therefore the transport coefficients can be connected with the largest positive Lyapunov exponent in the same way as known from the transport theory in relaxation time approximation.

The problem of irreversibility is one of the still open questions. Two approaches basically can be distinct. One approach considers the many particle theory as a suitable starting point to understand the increase of entropy as a result of many random collisions leading to irreversible kinetic equations like the Boltzmann equation. The other approach considers the theory of deterministic chaos with the characteristic measure of Lyapunov exponent to understand the occurrence of irreversibility. While the many particle approach can be easily extended to quantum systems the quantum chaos is still a matter of debate about the correct term.

If both approaches describe some facet of irreversibility, what we will anticipate in the following, it should be possible to give relations between them. While the characteristic measure of many body effects is the relaxation time and the transport coefficients, the relevant measure for chaotic systems is the Lyapunov exponent as a measure of phase space spreading of trajectories. Considerable efforts have been made to connect the transport coefficients with the Lyapunov exponent [1–4]. In [1,4] the fact, that the spreading of a small phase space volume is given by the sum of Lyapunov exponents $\delta V(t) = \delta V(0) \exp(\sum \lambda_i t)$, is used to give a relation between Lyapunov exponents and viscosity. This was possible to show with the help of the contact to a heat bath in the equation of motion ensuring constant internal energy. In [2,3] the relation between transport coefficients and Lyapunov exponents was presented in terms of Helfand's moments. The interlink was possible to establish by reinterpretation of the Helfand's moments as stochastic quantities such that the mean variance of the time derivatives represents just the transport coefficients. In [5] the authors derive a density expansion of largest Lyapunov exponent for hard sphere gases from a generalized Lorentz-Boltzmann equation. This demonstrated the intimate relation between transport coefficients and dynamical quantities like the Lyapunov exponent.

Here we like to show that there exists a very simple

connection between the concept of Lyapunov exponent and the dissipation leading to irreversibility for interacting Fermi systems. It will be shown that if the largest positive Lyapunov exponent is smaller than the product of Fermi velocity times wavelength in a Fermi system, the Lyapunov exponent appears in the same way as the relaxation time of the system. Therefore all expressions known from kinetic theory, expressing the transport coefficients in terms of the relaxation time, can be considered as an expression in terms of the Lyapunov exponent.

The concept of response of an interacting many body system starts conveniently from the distribution function $f(\mathbf{p}, \mathbf{r}, t)$ satisfying the appropriate kinetic equation, which by linearization yields the response to an external disturbance. First we discuss the quasiclassical response and generalize later to quantum response. The starting quasiclassical kinetic equation reads

$$\begin{aligned} \partial_t f(\mathbf{p}, \mathbf{r}, t) + \frac{\mathbf{p}}{m} \partial_{\mathbf{r}} f(\mathbf{p}, \mathbf{r}, t) \\ - \partial_{\mathbf{r}} (V_{\text{ind}}(\mathbf{r}, t) + V_{\text{ext}}(\mathbf{r}, t)) \partial_{\mathbf{p}} f(\mathbf{p}, \mathbf{r}, t) = \frac{f_0(\mathbf{p}, \mathbf{r}) - f(\mathbf{p}, \mathbf{r}, t)}{\tau} \end{aligned} \quad (1)$$

with the self-consistent mean-field potential given as a convolution between the two-particle interaction V_0 and the density $V_{\text{ind}} = \int d\bar{\mathbf{r}} V_0(\mathbf{r}, \bar{\mathbf{r}}) n(\bar{\mathbf{r}}, t)$, the external disturbance V_{ext} and a typical relaxation time τ . The relaxation time approximation serves here as the simplest form of collision integral to describe dissipative processes by internal collisions of the particles. This leads to a natural chaotization and ergodicity of the system.

Besides this chaotization by mutual collisions we want to discuss in the following how additional chaotic processes, e.g. caused by boundary conditions, surfaces etc., are influencing the response of the system to external perturbation V_{ext} .

When the equation (1) is linearized with respect to the external perturbation, the selfconsistent potential V_{ind} gives a linear density contribution δn via $\delta V_{\text{ind}} = V_0 \delta n$.

Defining the total polarization function as the connection between induced density variation and external perturbation

$$\delta n(\mathbf{x}, \omega) = \int d\mathbf{x}' \Pi(\mathbf{x}, \mathbf{x}', \omega) \delta V_{\text{ext}}(\mathbf{x}', \omega), \quad (2)$$

one finds the relation between the polarization function including the effect of the selfconsistent potential, Π , and the polarization without selfconsistent potential, Π_τ , as

$$\Pi(\mathbf{x}, \mathbf{x}') = \Pi_\tau(\mathbf{x}, \mathbf{x}') + \int d\bar{\mathbf{x}} d\bar{\mathbf{x}} \Pi_\tau(\mathbf{x}, \bar{\mathbf{x}}) V_0(\bar{\mathbf{x}}, \bar{\mathbf{x}}) \Pi(\bar{\mathbf{x}}, \mathbf{x}'). \quad (3)$$

In other words it is sufficient to concentrate on the response function Π_τ to an external potential without selfconsistent potential V_{ind} . The selfconsistent response Π is then given by the solution of the integral equation (3). The following derivation of Π_τ is adapted from [6].

Introducing the Lagrange picture by following the trajectory $\mathbf{x}(t), \mathbf{p}(t)$ of a particle

$$\begin{aligned} \frac{d}{dt} \mathbf{x} &= \frac{\mathbf{p}}{m} \\ \frac{d}{dt} \mathbf{p} &= -\partial_{\mathbf{x}} V_{\text{ext}} \end{aligned} \quad (4)$$

we linearize the kinetic equation equation (1) according to $f(\mathbf{x}, \mathbf{p}, t) = f_0(\mathbf{x}, \mathbf{p}) + \delta f(\mathbf{x}, \mathbf{p}, t)e^{-t/\tau}$ and obtain

$$\frac{d}{dt} \delta f(\mathbf{x}(t), \mathbf{p}(t), t) = \partial_{\mathbf{p}} f_0 \partial_{\mathbf{x}(t)} V_{\text{ext}}. \quad (5)$$

This can be integrated to yield

$$\begin{aligned} \delta f(\mathbf{x}, \mathbf{p}, t) &= \\ -2m \int_{-\infty}^0 dt' \int_{-\infty}^{\infty} d\mathbf{x}' \frac{d}{dt'} \delta(\mathbf{x}' - \mathbf{x}(t')) \frac{\partial f_0(p^2, \mathbf{x}')}{\partial p^2} V_{\text{ext}}(\mathbf{x}', t + t'). \end{aligned} \quad (6)$$

Integrating over \mathbf{p} , the density variation caused by varying the external potential is obtained as

$$\begin{aligned} \delta n(\mathbf{x}, \omega) &= -2mg \int d\mathbf{x}' \int \frac{d\mathbf{p}^3}{(2\pi\hbar)^3} \partial_{p^2} f_0(p^2, \mathbf{x}') \\ &\times \int_{-\infty}^0 dt' e^{-it'(\omega + \frac{i}{\tau})} V_{\text{ext}}(\mathbf{x}', \omega) \frac{d}{dt'} \delta(\mathbf{x}' - \mathbf{x}(t')) \end{aligned} \quad (7)$$

where g denotes the spin-isospin degeneracy. Comparing the expression (7) with the definition of the polarization function Π_τ in (2) and (3), we are able to identify the polarization of finite systems including the relaxation time as

$$\Pi_\tau(\mathbf{x}, \mathbf{x}', \omega) = \Pi_0(\mathbf{x}, \mathbf{x}', \omega + \frac{i}{\tau}) \quad (8)$$

with

$$\begin{aligned} \Pi_0(\mathbf{x}, \mathbf{x}', \omega) &= -2mg \int \frac{d\mathbf{p}^3}{(2\pi\hbar)^3} \partial_{p^2} f_0(p^2, \mathbf{x}') \\ &\times \int_{-\infty}^0 dt' e^{-it'\omega} \frac{d}{dt'} \delta(\mathbf{x}' - \mathbf{x}(t')). \end{aligned} \quad (9)$$

Further simplifications are possible if we focus on the ground state $f_0(p^2) = \Theta(p_f^2 - p^2)$ of the Fermi system. The modulus integration of momentum can be carried out and the Kirschnitz-formula [6,7] appears

$$\begin{aligned} \Pi_0(\mathbf{x}, \mathbf{x}', \omega) &= -\frac{mg p_f(\mathbf{x})}{4\pi^2 \hbar^3} \left[\delta(\mathbf{x}' - \mathbf{x}(0)) \right. \\ &\left. + i\omega \int_{-\infty}^0 dt' e^{-it'\omega} \int \frac{d\Omega_{\mathbf{p}}}{4\pi} \delta(\mathbf{x}' - \mathbf{x}(t')) \right]. \end{aligned} \quad (10)$$

This formula represents the ideal free part and a contribution which arises by the trajectories $\mathbf{x}(t)$ averaged over the direction at the present time $\mathbf{n}_p p_f = m\dot{\mathbf{x}}(0)$. In principle, the knowledge of the evolution of all trajectories is necessary to evaluate this formula. Molecular dynamical simulations can perform this task but it requires an astronomical amount of memory to store all trajectories. Rather, we discuss two approximations which will give us more insight into the physical processes behind. First the most radical one shows how the local density approximation emerges. In the next one we consider the influence of chaotic scattering.

The local density approximation appears from (10) when we perform two simplifications. Introducing Wigner coordinates $\mathbf{R} = (\mathbf{x} + \mathbf{x}')/2$, $\mathbf{r} = \mathbf{x} - \mathbf{x}'$ we have to assume

1. gradient expansion

$$p_f(\mathbf{R} + \frac{\mathbf{r}}{2}) \approx p_f(\mathbf{R}) + \mathcal{O}(\partial_{\mathbf{R}}) \quad (11)$$

2. expansion of the trajectories to first order history

$$\mathbf{x}' - \mathbf{x}(t') \approx -\mathbf{r} - t' \dot{\mathbf{x}} + \mathcal{O}(t'^2) = -\mathbf{r} - t' \frac{p_f}{m} \mathbf{n}_p. \quad (12)$$

With these two assumptions we obtain from (10) after trivial integrations

$$\begin{aligned} \Pi_0^{\text{LDA}}(\mathbf{q}, \mathbf{R}, \omega) &= \int d\mathbf{r} e^{-i\mathbf{q}\mathbf{r}} \Pi_0^{\text{LDA}}(\mathbf{r}, \mathbf{R}, \omega) \\ &= -\frac{m s p_f(\mathbf{R})}{4\pi^2 \hbar^3} \left\{ 1 + ik \int_0^\infty dy e^{iky} \frac{\sin y}{y} \right\} \end{aligned} \quad (13)$$

where $k = m\omega/(q p_f(\mathbf{R}))$. This can be further integrated with the help of

$$\begin{aligned}
& \int_0^\infty dy e^{iky} \frac{\sin y}{y} = \arctan(\text{Im } k - i \text{Re } k)^{-1} \\
& = 2i \ln \left(\frac{1+k}{1-k} \right) + \pi [\text{sgn}(1+k) + \text{sgn}(1-k)] \Big|_{\text{Im } k \rightarrow 0} \quad (14)
\end{aligned}$$

to yield the standard Lindhard result (27) in the classical limit

$$\begin{aligned}
\Pi_0^{\text{inf}}(\mathbf{q}, p_f, \omega) = & -\frac{m g p_f}{4\pi^2 \hbar^3} \left\{ 1 - 2k \ln \left(\frac{1+k}{1-k} \right) \right. \\
& \left. + ik\pi [\text{sgn}(1+k) + \text{sgn}(1-k)] \right\} \quad (15)
\end{aligned}$$

where $k = m\omega/(qp_f)$. We recognize the ground state result for infinite matter except that the Fermi momentum $p_f(\mathbf{R})$ has to be understood as a local quantity corresponding to local densities so that we get with (8)

$$\Pi_\tau^{\text{LDA}}(\mathbf{q}, \mathbf{R}, \omega) = \Pi_0^{\text{inf}}(\mathbf{q}, p_f(\mathbf{R}), \omega + \frac{i}{\tau}). \quad (16)$$

For extensions beyond the local density approximation see [7,8].

Now we focus on the influence of an additional chaotic scattering which will be caused e.g. by a surface boundary. In order to investigate this effect we add to the regular motion (12) a small irregular part $\Delta \mathbf{x}$

$$\mathbf{x}' - \mathbf{x}(t') \approx -\mathbf{r} - t' \frac{p_f}{m} \mathbf{n}_p + \Delta \mathbf{x}. \quad (17)$$

The irregular part of the motion we specify in the direction of the current movement lasting a time Δ_t and given by an exponential increase in phase-space controlled by the largest Lyapunov exponent λ . Therefore we can assume [$t' < 0$]

$$\Delta \mathbf{x} \approx \frac{p_f \mathbf{n}_p}{m} \Delta_t \exp[-\lambda(t' - \Delta_t)] + \text{const.} \quad (18)$$

Since we are looking for the largest Lyapunov exponent we can take (18) at the maximum $\Delta_t = -1/\lambda$. Further, we require, that in the case of vanishing Lyapunov exponent we should regain the regular motion (12). We have for (17) therefore

$$\mathbf{x}' - \mathbf{x}(t') \approx -\mathbf{r} - \frac{p_f}{m} \mathbf{n}_p \left[\frac{1 - \exp(-\lambda t')}{\lambda} \right]. \quad (19)$$

With this ansatz one derives from (10) instead of (13) the result

$$\begin{aligned}
\Pi_\lambda(\mathbf{q}, \mathbf{R}, \omega) = & -\frac{m g p_f(\mathbf{R})}{4\pi^2 \hbar^3} \\
& \times \left[1 + ik \int_0^\infty dy \frac{\sin y}{y} \left(1 + \frac{ky}{\omega} \lambda \right)^{i\omega/\lambda - 1} \right], \quad (20)
\end{aligned}$$

which for $\lambda \rightarrow 0$ resembles exactly (13). The further integration could be given in terms of hypergeometric functions but this is omitted here.

With this formula together with (8) and (3) we have derived the main result of a polarization function including the influence of many particle effects and additional chaotic process characterized by the Lyapunov exponent λ .

For the condition

$$\lambda \ll qv_F \quad (21)$$

with $v_f = p_f/m$ the Fermi velocity and q the wave length we can use $\lim_{x \rightarrow \infty} (1 + a/x)^x = \exp(a)$ under the integral of (20) and the final integration is performed with the result of (16) but a complex shift

$$\Pi_\lambda^{\text{LDA}}(\mathbf{q}, \mathbf{R}, \omega) = \Pi_0^{\text{inf}}(\mathbf{q}, p_f(\mathbf{R}), \omega + i(\lambda + \frac{1}{\tau})). \quad (22)$$

We obtain by this way just the known Matthiessen rule which states that the damping mechanisms are additive in the damping $\Gamma = \frac{1}{\tau} + \lambda$.

Next we discuss the quantum response function and we will see that all discussions outlined above can be straight forward applied to the quantum response function. Instead of the quasiclassical kinetic equation (1) we start now from the quantum kinetic equation [9]

$$\begin{aligned}
& \partial_t f(\mathbf{p}, \mathbf{r}, t) + \frac{\mathbf{p}}{m} \partial_{\mathbf{r}} f(\mathbf{p}, \mathbf{r}, t) - \frac{1}{i} \int d\mathbf{s} \frac{d\mathbf{p}'}{(2\pi\hbar)^3} \left[U(\mathbf{r} + \frac{\mathbf{s}}{2}) \right. \\
& \left. - U(\mathbf{r} - \frac{\mathbf{s}}{2}) \right] e^{\frac{i}{\hbar} \mathbf{s}(\mathbf{p}' - \mathbf{p})} f(\mathbf{p}', \mathbf{r}, t) = \frac{f_0(\mathbf{p}, \mathbf{r}) - f(\mathbf{p}, \mathbf{r}, t)}{\tau} \quad (23)
\end{aligned}$$

with $U = V_{\text{ind}} + V_{\text{ext}}$. The gradient expansion in U leads to first order the quasiclassical expression (1). We follow now exactly the same linearization as above and introduce the Langrange picture. The trajectories are now described instead of (4) by the following set

$$\begin{aligned}
& \frac{d}{dt} \mathbf{x} = \frac{\mathbf{p}}{m} \\
& \mathbf{s} \frac{d}{dt} \mathbf{p} = U(\mathbf{r} + \frac{\mathbf{s}}{2}) - U(\mathbf{r} - \frac{\mathbf{s}}{2}) \quad (24)
\end{aligned}$$

where the arbitrary vector \mathbf{s} shows the infinite possibilities of trajectories by quantum fluctuations. The resulting polarization function for a finite quantum system reads now instead of (8)

$$\begin{aligned}
\Pi_0(\mathbf{x}, \mathbf{x}', \omega) = & \frac{g}{\pi^2 \hbar^3} \int \frac{d\mathbf{p}}{(2\pi\hbar)^3} \int d\mathbf{s} \frac{\sin(\frac{1}{\hbar} \mathbf{s} \mathbf{p})}{s} \\
& \times \partial_s \left(\frac{\sin(\frac{1}{\hbar} \mathbf{s} p_f)}{s} \right) \int_{-\infty}^0 dt' e^{-it'\omega} \delta(\mathbf{x}' - \mathbf{x}(t') - \frac{\mathbf{s}}{2}). \quad (25)
\end{aligned}$$

Compared with (9) we see that due to quantum fluctuations an additional integration \mathbf{s} appears. Eq. (25) is the

quantum generalization of the quasiclassical Kirschnitz formula (10) for the response function in finite systems.

Applying now the same gradient approximation (12) we derive from (25) with the help of

$$i \int d\mathbf{s} \frac{\sin(\frac{1}{\hbar}\mathbf{s}\mathbf{p})}{s} \partial_s \left(\frac{\sin(\frac{1}{\hbar}s p_f)}{s} \right) e^{i\frac{1}{2}\mathbf{q}\mathbf{s}} = \pi^2 \hbar^3 \left[\Theta(p_f^2 - (\mathbf{p} - \frac{\mathbf{q}}{2})^2) - \Theta(p_f^2 - (\mathbf{p} + \frac{\mathbf{q}}{2})^2) \right] \quad (26)$$

the quantum Lindhard result

$$\Pi_0(\mathbf{q}, \mathbf{R}, \omega) = g \int \frac{d\mathbf{p}}{(2\pi\hbar)^3} \frac{\Theta(p_f^2(\mathbf{R}) - (\mathbf{p} - \frac{\hbar\mathbf{q}}{2})^2) - \Theta(p_f^2(\mathbf{R}) - (\mathbf{p} + \frac{\hbar\mathbf{q}}{2})^2)}{\hbar\omega - \frac{\hbar\mathbf{p}\mathbf{q}}{m} + i\epsilon} \quad (27)$$

in local density approximation.

The ansatz about additional chaotic processes (19) leads then to exactly the same expression (22) under the condition (21) but with the quantum response (27) instead of Π_0^{inf} .

We like to point out that this result has far reaching consequences. With the assumption (21) we have shown by this way that the linear response behavior is the same if dissipation comes from the relaxation time via collision processes in many - particle theories or from the concept of chaotic processes characterized by the Lyapunov exponent. We can therefore state that for small Lyapunov exponent compared to the product of wave length and Fermi velocity in a many particle system, the largest Lyapunov exponent behaves like the relaxation time in the response function.

Since the transport theory is well worked out to calculate the transport coefficients in relaxation time approximation we can express by this way the transport coefficients in terms of the Lyapunov exponent alternatively. This illustrates the mutual equivalence of the concept of Lyapunov exponent and dissipative processes in many-particle theories.

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